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THERMAL ANALYSIS OF HIGH LEVEL WASTE GEOLOGICAL DISPOSAL MODULE WITH THE THERMAL CODE SYRTHES

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ABSTRACT

Within the framework of the 2006 French law on sustainable management of radioactive materials and waste, an evaluation of the industrial perspectives of GENERATION IV Fast Reactors deployment is requested for 2012. In this context, questions about waste storage capacities are of interest for EDF (Electricité de France). The storage area is driven by thermal requirements on the argillite formation surrounding the canisters. The size of the final radioactive waste geological repository is one indicator of interest in these studies. The repository considered has been proposed by ANDRA, the French national agency in charge of the radioactive waste management. Optimisation studies on the number of canisters per cell or the distance between two cells using the open source thermal code SYRTHES and SALOME have been presented in previous conferences. However, due to the very large number of calculations induced they are performed on a limited domain. To evaluate the thermal conservatism of a reduced domain, three levels of modeling have been used : a domain limited to half a cell, a slice of half a module (ie three half cells), and a complete half module leading to a very large finite element model (more than 82 million cells), in which all the disposal cells (around 150 of them containing 6 waste packages each) are represented. Two theoretical heat deposit functions have been used representative of waste leading to early and late temperature peaks. This paper presents the thermal code SYRTHES used to simulate large model for transient lasting up to 4000 years. Results show that clay temperature surrounding cells located on the periphery are cooler than those located near the center of the module. For early peaks a reduced domain is well adapted for optimization studies, while for late peak wastes, taking into account an extended domain seems interesting since the large case underlines that optimizing on a reduced domain is clearly conservative.

INTRODUCTION

As exposed in [1,2] the minimization of high level long lived radioactive waste is one of Generation IV objectives, as well as an optimal use of uranium resources. Different scenarios regarding the transmutation of minor actinides have been investigated. They may have an impact on the deep geological disposal size and therefore on the cost associated.

Scenario simulation studies are presently done at EDF with the code TIRELIRE-STRATEGIE to investigate the operation of a nuclear fleet and the impact it may have on the fuel cycle facilities (see [1,2]). That code computes the nuclear material fluxes at all steps of the nuclear fuel cycle, including the back-end of the cycle with the high level waste (HLW) glass canisters production, but a thermal repository model is still required. This thermal aspect is handled thanks to the open source thermal code SYRTHES (see [3,4]), developed at EDF. It is used to simulate the thermal behavior of the glass canister and the surrounding clay. The glass power is modeled through a sum of exponentials corresponding to the contribution of the main isotopes. In the present paper, two theoretical glass power are used: the first kind could correspond to canisters coming from the reprocessing of PWR-UOX assemblies and lead to a temperature peak arising shortly after the start. The second one could illustrate a canister coming from the reprocessing of SFR-MOX assemblies and characterized by an important contribution of Americium to the thermal residual power, and leads to a late temperature peak. The repository concept studied is the one proposed by ANDRA (see [6]), the French National Agency in charge of the radioactive waste management, but the methodology could be applied to other concepts.

THE THERMAL MODEL (ANDRA DESIGN)

This paragraph gives a rapid overview of the ANDRA design (see [6]). The underground disposal facility consists of disposal cells excavated in an argillite formation at a depth of about 500 m and containing the waste packages (vitrified glass canisters, since scenarios of complete spent fuel recycling are investigated). As shown in the Fig. 1 (taken from ANDRA reports), disposal cells are located in parallel horizontal tunnels disposed in a comb structure, around access drifts:

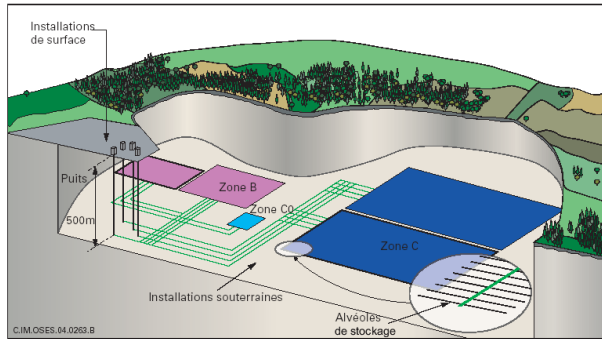


Fig. 1. Organisation of the repository (ANDRA)

Fig 2. presents a High Level Waste (HLW) repository located in an argillite layer (Callovo-Oxfordien) surrounded by other layers with different thermal properties. The horizontal structure leads to orthotropic thermal behaviour (with vertical thermal conductivities being less than the horizontal ones).

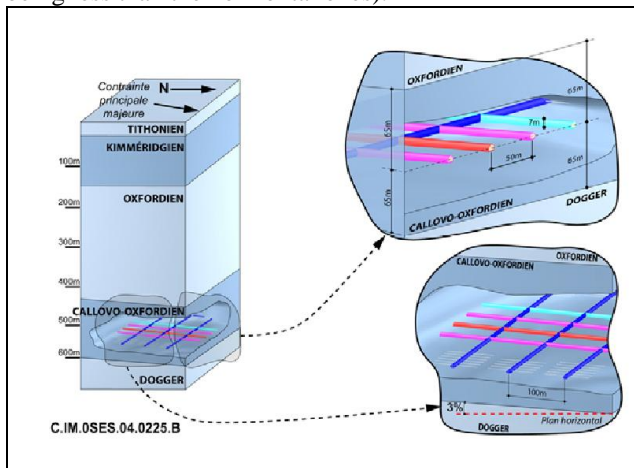


Fig. 2. Detailed view of the repository in the Callovo-Oxfordien layer (ANDRA)

Fig. 3 presents a closer view of a module containing access drifts and hundreds of disposal cells. The dash lines underlines the symmetry which will be used in the calculations.

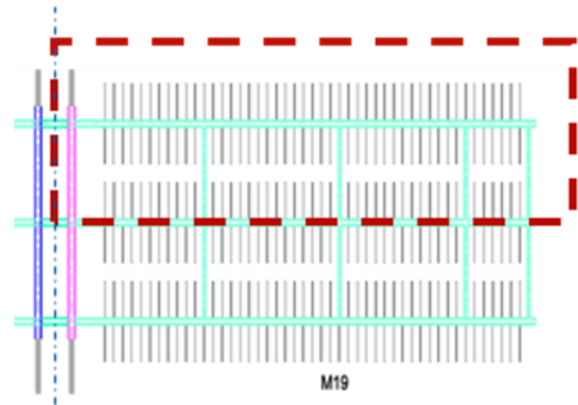


Fig. 3. Module (ANDRA)

HLW disposal cells are dead end, horizontal bore-holes with an excavated diameter of around 0.7 meter. They are equipped with a metallic sleeve which supports the argillite and enables package handling for their introduction and positioning, and also a possible retrieval (see Fig. 4). Their length is about 40 meters, but only the end part is used for package disposal. Each disposal cells contains a single row containing up to 18 waste packages, depending on their thermal load.

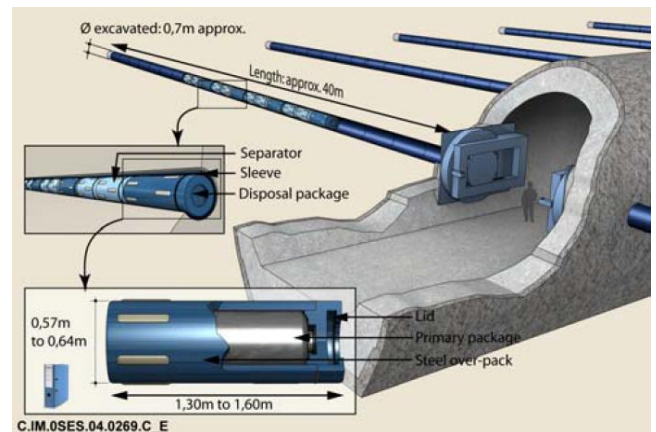


Fig. 4. Vitrified disposal cell . (ANDRA)

Dummy glass packages are inserted between waste packages to dilute the impact of waste canisters energy release on the surrounding clay. Their length is adjusted to respect temperature criteria of 90°C in the clay.

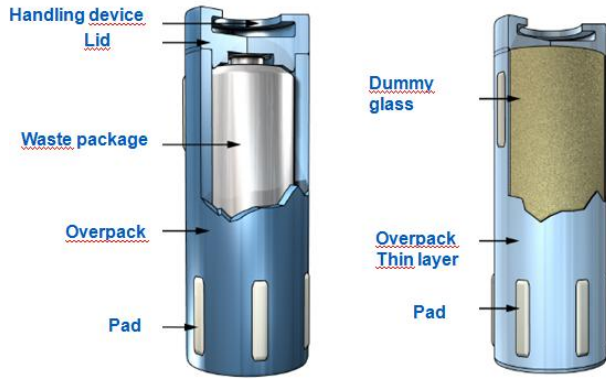


Fig. 5. Waste package (left) and separator (right) (ANDRA)

Waste packages and dummy glass packages inside the waste cell are separated from the metallic sleeve by supporting pads disposed all around the steel envelope (see Figs. 5 and 6).

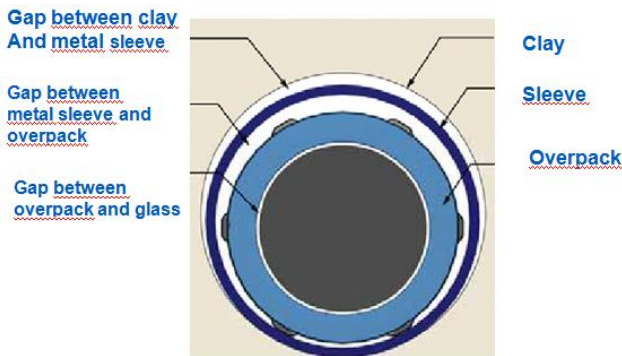


Fig. 6. Vertical cross section of waste package in cell (ANDRA)

THE THREE MODELS CONSIDERED

In this paper we are not interested to perform an optimization study like in [1,2], but investigate the domain extension influence. Therefore the number of waste packages has been arbitrarily fixed to 6 per cell and the distance between two cells corresponds to the ANDRA design presented on Fig. 3 (about 13.5m). Three domains have been considered:

- The first one corresponds to only half a cell (similar to what is used for optimization purpose (see [1,2]) thanks to SYRTHES [3,4] and SALOME[5]).
- The second one to half a slice of module (ie 3 half cells), which enables us to take into account the inter module distance. This kind of model is also used for optimization studies performed for late peak waste (see [2]).
- The last and bigger one corresponds to half a module (see Fig 3). This case is used to perform an optimization study but identify for a given theoretical waste how conservative in terms of temperature reached, limited domain can be.

THE THERMAL CODE SYRTHES

This chapter presents briefly the thermal code SYRTHES developed at EDF. Writing the energy conservation in a solid leads to :

$$\rho C_p \frac{\partial T}{\partial t} = \text{div} (k_s \overrightarrow{\text{grad}} T) + \Phi \quad (1)$$

In the above equation, T is the temperature, t the time, Φ a volumetric source or sink, ρ and C_p respectively the density and the specific heat. All these quantities may vary with respect to time and space. Finally k_s designates the conductive behavior of the medium. k_s is reduced to a scalar (still variable in time and space) when the material is considered isotropic, but materials (for example argillite layers), may exhibit behaviors in which the flux is not aligned with the temperature gradient. Then, the conductivity matrix (always considered symmetrical) contains up to 3 coefficients in 2D and up to 6 in 3D (reduced respectively to 2 and 3, when aligned with the coordinates axis)

In order to solve equation (1), a finite element approach is used. It allows a good description of complex geometries at reasonable cost. For optimization reasons, only two kinds of elements have been retained in SYRTHES : 3 nodes triangles in 2D and 4 nodes tetrahedra in 3D.

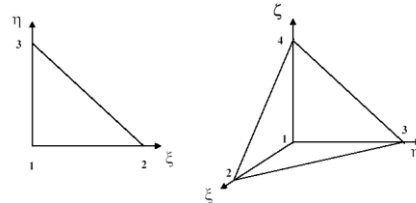


Fig. 7 : Elements retained in SYRTHES

The spatial discretization is of P1 type, which means that variables vary linearly between two adjacent nodes belonging to each element on the sketch of Fig. 7 (for 2D and 3D cases). This choice has been motivated by the advantages it provides when evaluating elementary matrices as it is pointed out in the next section. Using a weak formulation and the Galerkin method, the following system of the differential equations can be derived in which v is a test function, Ω is the space, and Γ the boundary.

$$\forall v \in V \quad \int_{\Omega} \frac{\rho C_p}{\delta t} (T^{n+1} - T^n) v d\Omega = - \int_{\Omega} k_s \overrightarrow{\text{grad}} T^{n+1} v d\Omega + \int_{\Gamma_q} q^n v d\Gamma_q + \int_{\Omega} \Phi^n v d\Omega \quad (2)$$

Basically, in equation (2), two kinds of elementary matrix have to be evaluated. One is of the mass type, and the other comes from the diffusion operator. These elementary matrices can be calculated by classical Gauss quadrature methods, but it interesting to notice that their calculation can also be carried out analytically because of the simple expression they take for the chosen elements. Typically for a

constant physical property per element, geometrical consideration shows that elementary mass matrices are only related to the area of the triangle in 2D and the volume of the tetrahedron in 3D. Let φ be a shape function, S and V respectively the area and the volume of the triangle and the tetrahedron, then the mass matrices take the following forms :

$$\int_Q \varphi_i \varphi_j dS = \frac{S}{12} \begin{pmatrix} 2 & 1 & 1 \\ & 2 & 1 \\ & & 2 \end{pmatrix} \quad (3)$$

$$\int_Q \varphi_i \varphi_j dV = \frac{V}{20} \begin{pmatrix} 2 & 1 & 1 & 1 \\ & 2 & 1 & 1 \\ & & 2 & 1 \\ & & & 2 \end{pmatrix} \quad (4)$$

Regarding the diffusion terms, they are evaluated as in Eq. (5) when one considers that due to the nature of the retained elements, the gradients on elements are constant.

$$\int_{\Omega_e} k_s \overrightarrow{\text{grad}}\varphi_i \overrightarrow{\text{grad}}\varphi_j d\Omega_e = k_s \overrightarrow{\text{grad}}\varphi_i \overrightarrow{\text{grad}}\varphi_j \int_{\Omega_e} d\Omega_e \quad (5)$$

Classical boundary conditions (Dirichlet, heat exchange, flux, ...) are evaluated thanks to boundary integrals. Then the system is solved by a conjugated gradient (preconditioned by the assembled diagonal) well adapted to symmetrical matrices. Numerous validations against analytical solutions have been performed.

MESH GENERATION

In order to compute the thermal aspects, one needs to generate a grid for conduction (tetrahedra). This step is generally time consuming. Fig. 8 and 9 present the meshes in which materials with different thermal behaviour have been given different colours (for example the different argillite layers, concrete, metal, glass, ...). In this reference case, the access drift is explicitly represented as well as a complete disposal cell containing here 6 HLW packages. One underlines that this geometry does not correspond to a thermal optimization step for the waste package considered.

Fig. 8 presents a view around the cell region, but the domain simulated extends from 500 m above (ie up to the ground surface) and 500 m below that layer. The corresponding mesh counts about 700000 tetrahedra, a previous mesh sensitivity study has proved that such a refinement is fine enough to capture all the thermal phenomena during the very long transient.

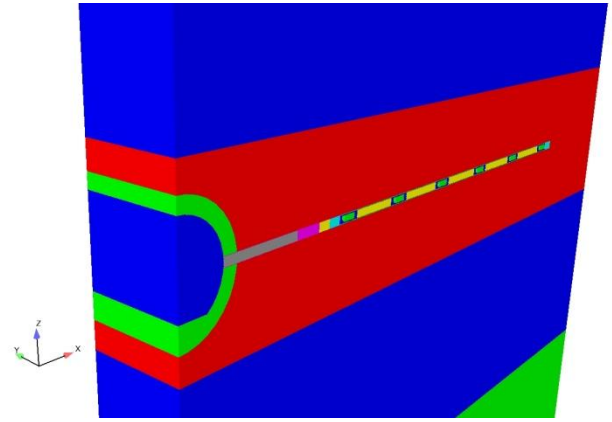


Fig. 8 : General view of the cell (with 6 packages)

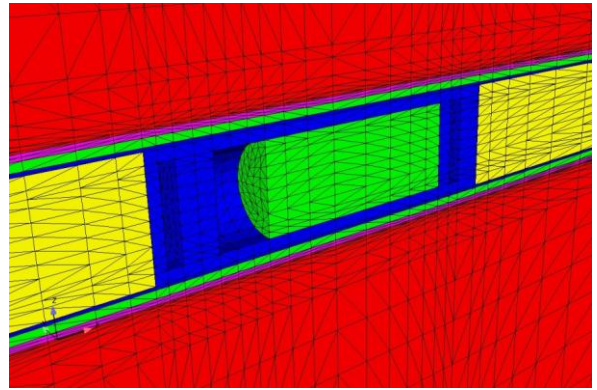


Fig. 9 : Detailed view of a waste package

The spatial discretization of the waste package itself can be seen on Fig. 9. The vitrified waste is represented in green and represents a volume of around 0.114 m^3 . The empty extremity of the package corresponds to the fact that the primary waste package is not completely filled with glass and leaves an empty space of around 20 cm. Likewise a space corresponding to a gap in the lead is also represented. The blue part represents the highly conductive stainless steel of the over-pack and the yellow domain corresponds to the dummy glass.

The second mesh generated (see Fig. 10) corresponds to a slice of a module containing three cells (containing 6 HLW packages each). To remove a possible spatial discretisation bias, we used exactly the same spatial discretisation as before, leading to a mesh three times bigger. This mesh includes inter-module additional ground (back of Fig. 10).

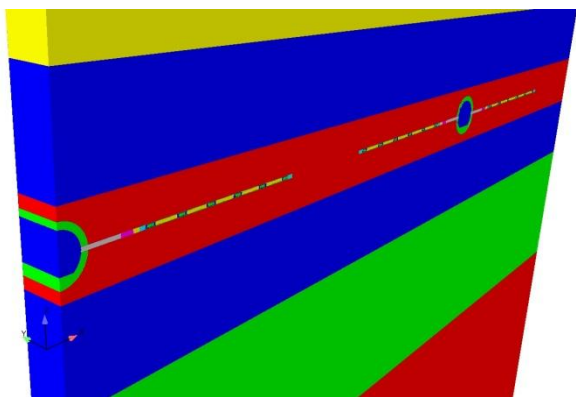


Fig. 10 : Global view of a module slice

Generating the mesh corresponding to the full half module case (containing hundreds of cells with 6 HLW each) is much more challenging. Due to the repeated pattern, it has been built by block, then reassembled as shown on Fig. 11 presenting a detailed view of the horizontal plane containing all the cells and the horizontal access drifts.

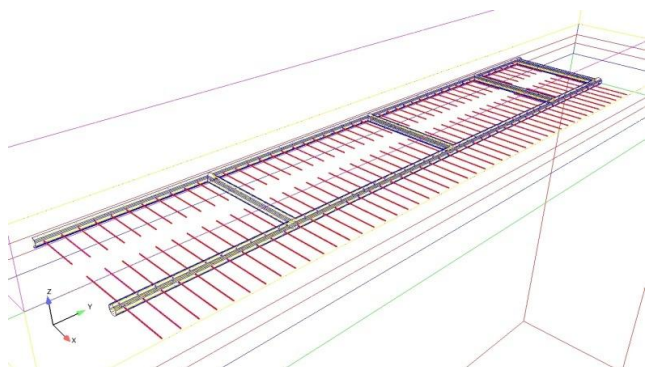


Fig. 11 : Half a module mesh (82 million tetrahedra)

However, due to the very long transient we have to handle, we have sought to reduce the global number of cells without changing the spatial discretization near the region of interest. To do so, we have used the same mesh for cells where we expect maximum temperature and used a coarser mesh far from the region of interest and have made sure that the thermal effect stays the same. This enables us to reduce the number of cells from around 230 million tetraedra down to 82 million. For that still big case, the domain is then split in a number of independent parts containing a well balanced number of elements thanks to METIS software (see [7]). Fig. 12 shows the number of tetraedra per domain while Fig. 13 shows a graphical view of the partitioned mesh. Calculations have been performed on clusters with 32 processors up to 256 processors using the parallel version of SYRTHES relying on MPI [8].

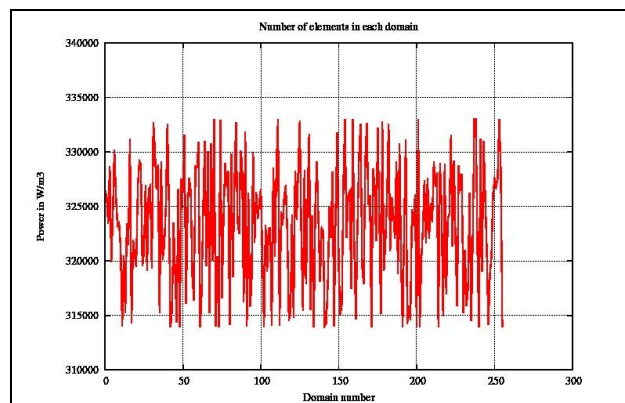


Fig. 12 : Distribution of the number of element per part

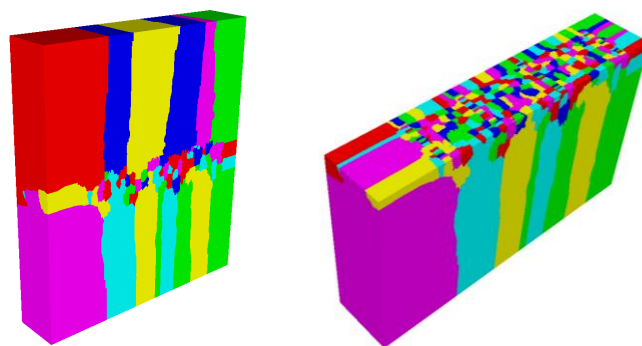


Fig. 13 : Splitting the domain in 256 parts thanks to METIS (each part is treated by a processor)

For the three models, two kinds of meshes have been generated: one valid during the 30 first years for which a ventilation can be set through the access drifts, and a second one when access drifts are filled with ground material (this operation takes place after 30 years at temperature of 25°C)

MATERIALS PROPERTIES

All material properties can be found in ANDRA documents (see [6]). Thermal behaviour is considered isotropic apart for the Callovo-Oxfordien layers for which an orthotropic conductivity function of temperature is set respectively for the three Callovo-oxfordien layers.

Other material properties (density, heat capacity and conductivity) are considered isotropic but still depend of the local temperatures. The heat transfer between the over-pack and the sleeve is done through an equivalent conductivity (see eq 5) taking into account thermal radiation.

$$\lambda_{equivalent} = \frac{\varepsilon_1 \varepsilon_2}{1 - (1 - \varepsilon_1 R_1 / R_2)(1 - \varepsilon_2)} \sigma (T_1^2 + T_2^2)(T_1 + T_2) R_1 \log \left(\frac{R_2}{R_1} \right) \quad (5)$$

Regarding initial conditions, at time $t=0$ of the simulation a vertical geological temperature profile is set with respect to the depth and adiabatic condition is set on the domain boundary.

According to the HLW packages the heat deposit varies. Two theoretical residual heat deposit functions (in W/m^3) in

the glass with respect to time (in years) are plotted on Fig. 14.

- The green curve could correspond to a generic HLW package coming from the reprocessing of UOX assemblies exhibiting a strong decrease quite rapidly.
- The red curve could correspond to typical HLW package produced by the reprocessing of a GenIV SFR MOX (including an important part of Americium) which explains why the decrease is less pronounced.

One underlines that the main point here is the shape of these theoretical curves and not the absolute values. Both curves decrease but not at the same rate. Therefore the thermal equilibrium between the heat released and the heat possible to be evacuated through the clay is not the same.

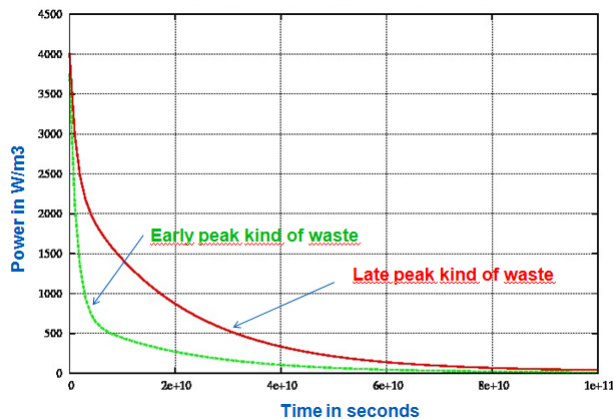


Fig. 14 : Heat deposit in the glass (for two kinds of waste)

MODEL IMPACT ON AN EARLY PEAK WASTE.

Fig. 15 shows the temperature field obtained after 30 years for a “realistic” boundary condition (ie $h=5 \text{ W/m}^2/\text{°C}$ in the access drift and adiabatic in the head of the cell).

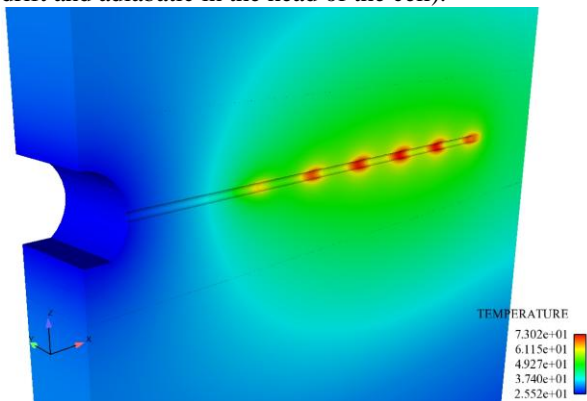


Fig. 15 : Clay temperature field obtained after 30 years

The same calculation has been performed with the second model (slice of a module) and is shown on Fig. 16. Clearly, the three cells do not exhibit the same temperature due to the influence of the inter module ground (right of the image) which gives an additional thermal inertia and the possibility to increase heat loss.

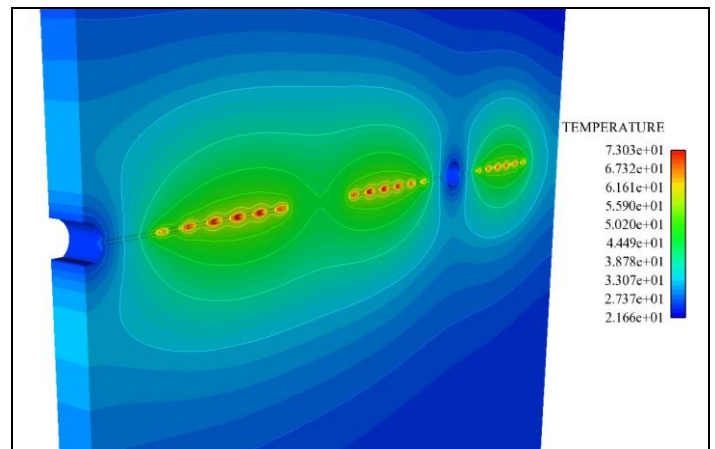


Fig 16 : Clay temperature field (in °C) after 30 years

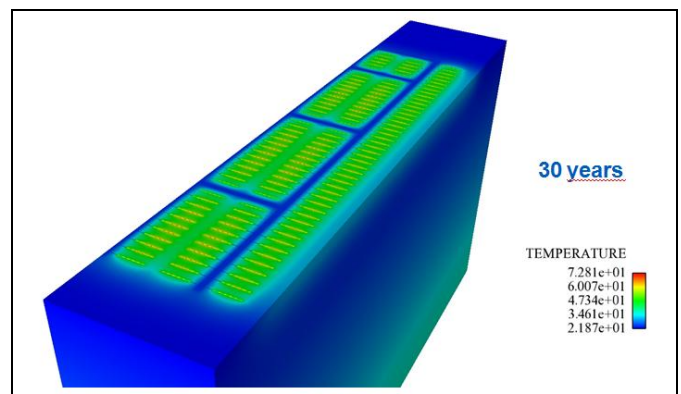


Fig. 17 : Clay temperature field (in °C) after 30 years

Table 1 : Maximum temperature reached (around 12.5 years)

	½ cell	½ slice of module	½ module
Glass	120.64 °C	120.64 °C	120.60 °C
Over-pack	93.20 °C	93.20 °C	93.12 °C
Clay	77.55 °C	77.55 °C	77.44 °C

As was expected the three different models provide the same peak temperature (see table 1) for an early peak kind of waste package, simply because after 12 years, even on the reduced domain, boundary conditions are not yet affecting the maximum temperature. The calculation has then been continued after the filling of the access drift for the three models from 30 years after the start until 4000 years. Fig. 18 shows the longitudinal temperature profile at a location where highest temperatures are found. Initially, the HLW packages are quite hot compared to the surrounding clay, but as time goes by, the temperature profiles becomes smoother and smoother to end by an almost flat profile at 4000 years.

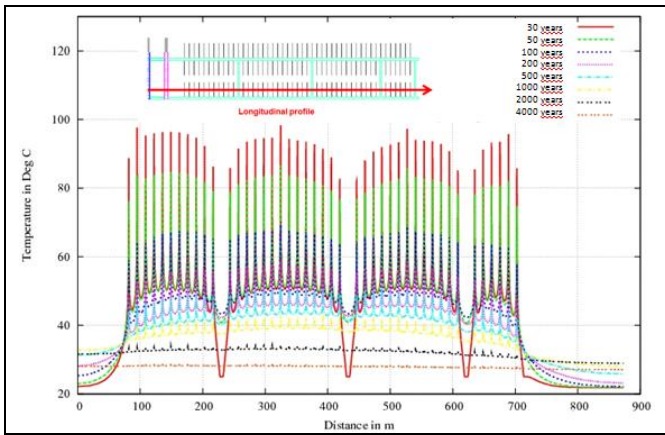


Fig. 18 : Longitudinal temperature profile (located in the middle of the module) after 30,50, 100, 200, 500, 1000 2000 and 4000 years.

Fig. 19 to 22 show the same aspect through the thermal field when keeping a constant temperature scale varying between 20°C and 70°C. As is clearly seen the temperature reaches a peak at first and decreases quite fast.

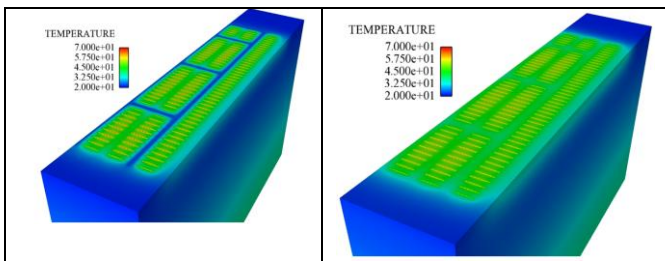


Fig. 19 : T in (°C) at 30 years (left) and 50 years (right)

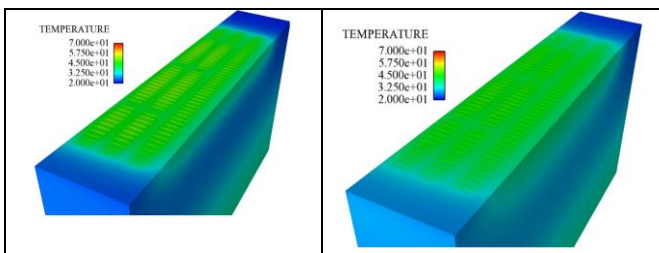


Fig. 20 : T in (°C) at 100 years (left) and 200 years (right)

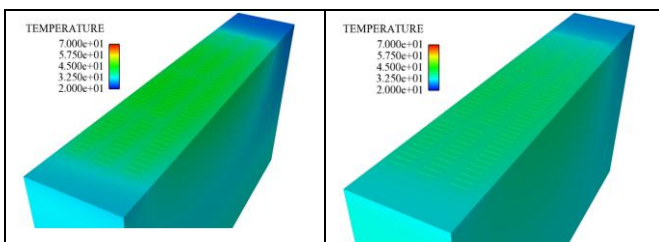


Fig. 21: T in (°C) at 500 years (left) and 1000 years (right)

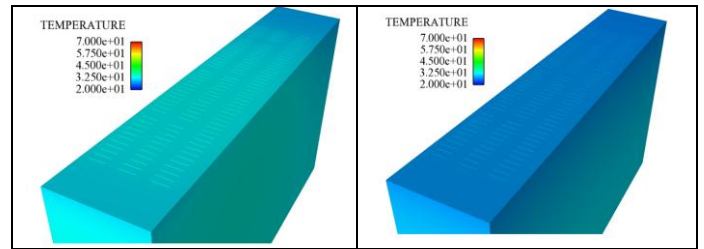


Fig. 22:T in (°C) at 2000 years (left) and 4000 years (right)

Highlighting the spatial non uniformity.

Here one wants to underline that at each stage, the temperature field is non uniform from one storage cell to another. Cells located in the periphery of the module are cooler than those located near the center of the module.

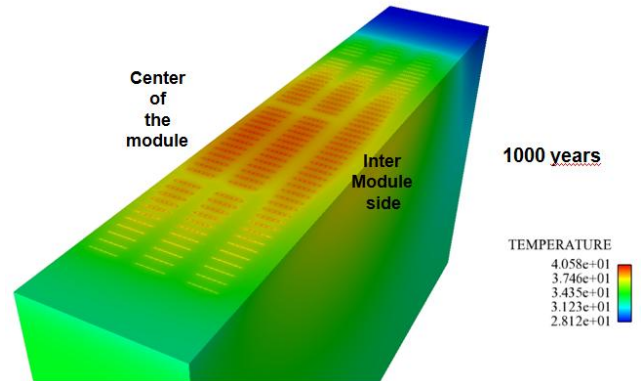


Fig. 23 : Zoom on temperature field in the clay after 1000 years. Beware that temperature scale is here adapted to a narrow range [28°C to 41°C] to highlight the temperature spatial non uniformity even at 1000 years

More quantitatively, one can plot the longitudinal and transversal profiles through the module at 1000 years.

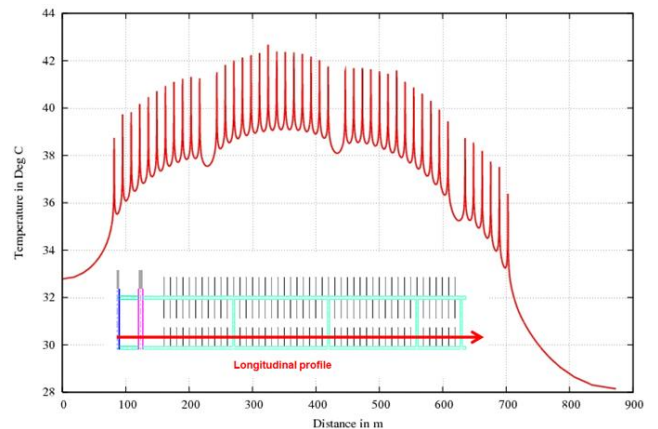


Fig. 24 : Longitudinal temperature profile (cutting the waste packages with highest temperatures) after 1000 years

To illustrate the same non uniformity aspect, two transversal profiles have been plotted on Fig. 25.

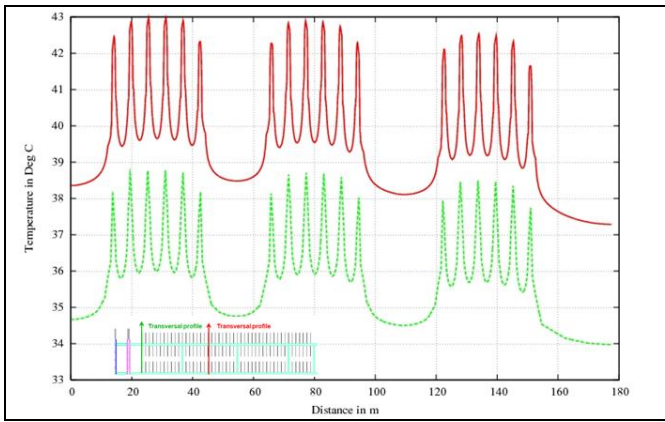


Fig. 25 : Transversal temperature profiles (central storage cell in red and periphery storage cell in green)

Comparison of maximum temperature

Fig. 26 to 28 show the maximum temperature found respectively in the glass, over-pack and clay for the three models (blue for 1/2 cell, green for half slice, red for half volume) during the transient. On all curves, a steep temperature decrease can be observed, illustrating that after filling of the access drifts, clay evacuates heat faster than what the HLW packages provide.

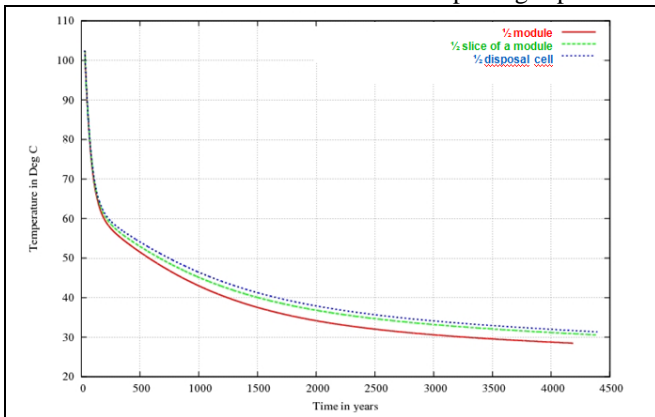


Fig. 26 : Maximum temperature evolution in the glass

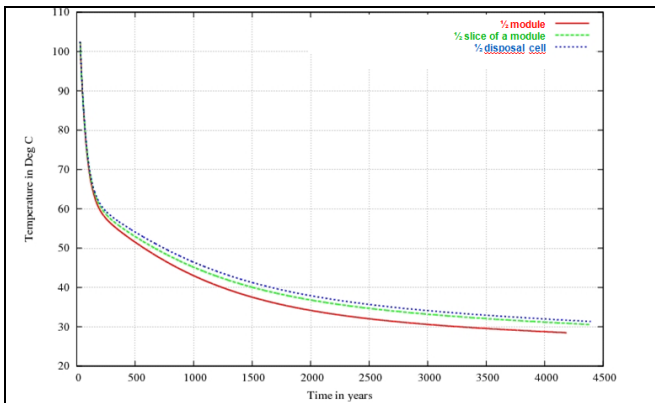


Fig. 27 : Maximum temperature evolution in over-pack

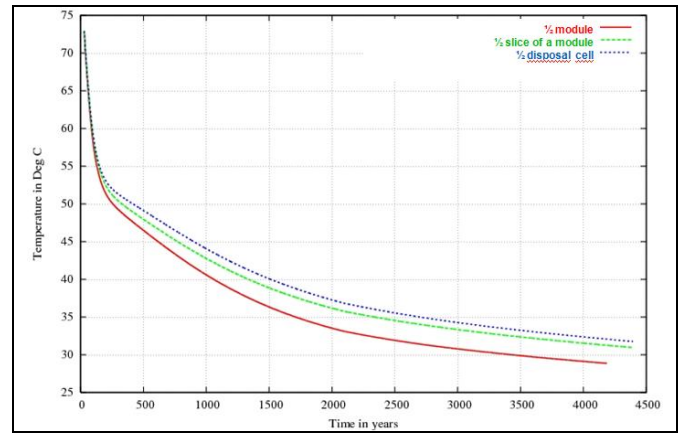


Fig. 28 : Maximum temperature evolution in the clay

MODEL INFLUENCE ON A LATE PEAK WASTE.

A similar study is performed for the SFR kind of waste package. Due to the contribution of the isotopes, the peak is then arising much later. Similar views (temperature between 20°C and 90°C) are shown below:

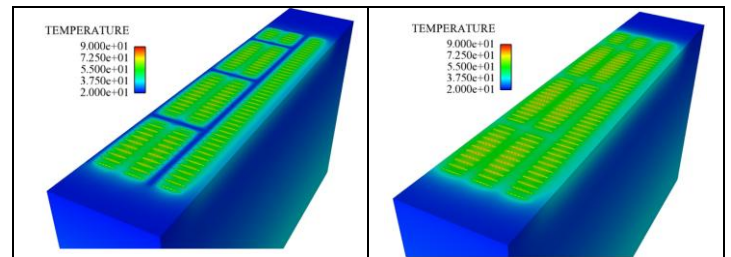


Fig. 29 : T in (°C) at 30 years (left) and 50 years (right)

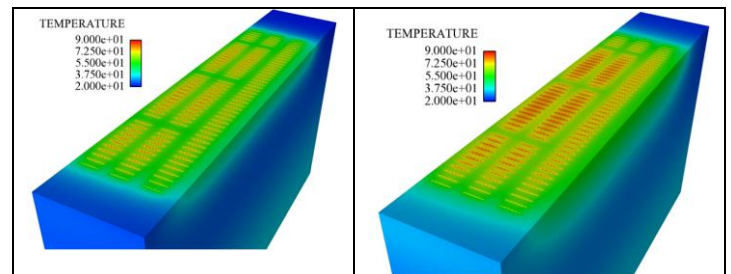


Fig. 30 : T in (°C) at 100 years (left) and 200 years (right)

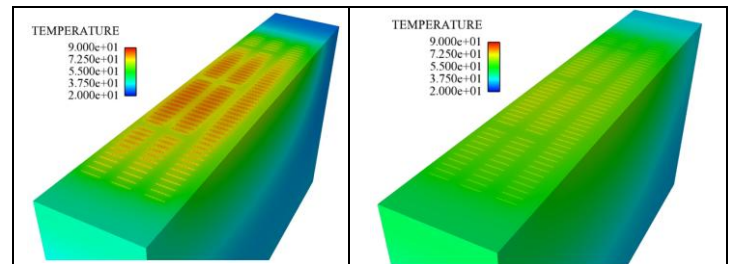


Fig. 31 : T in (°C) at 500 years (left) and 1000 years (right)

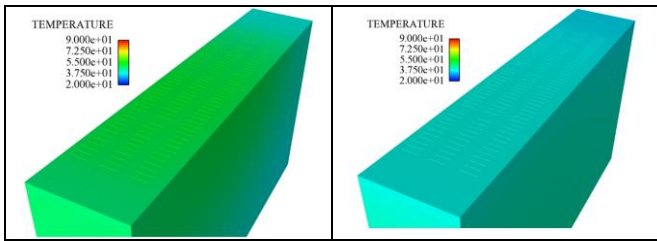


Fig. 32 : T in °C at 2000 years (left) and 4000 years (right)

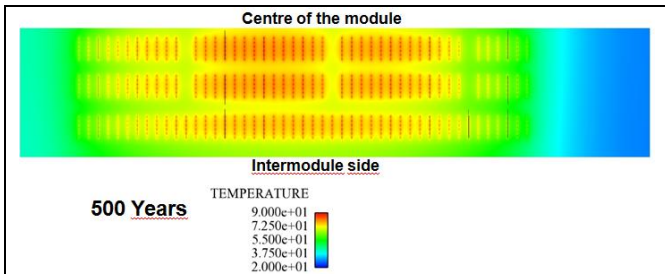


Fig. 33 : Temperature field in the clay (horizontal plane cutting the disposal cells) after 500 years

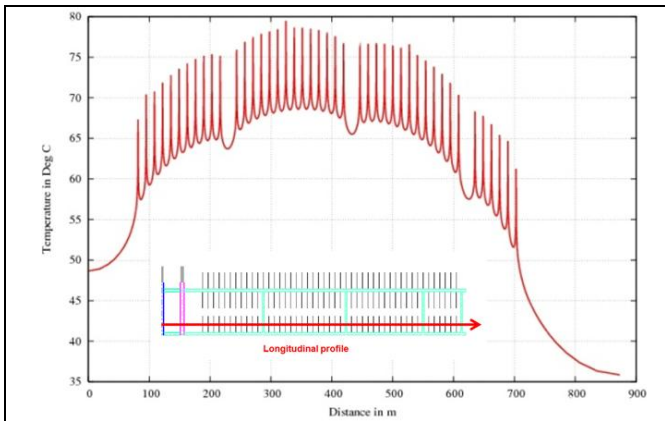


Fig. 34 : Longitudinal temperature profile (cutting the waste packages with highest temperatures) after 1000 years. The peak correspond to the different cells.

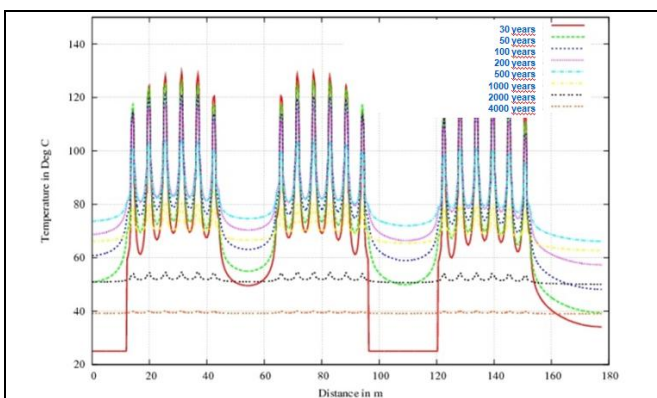


Fig 35. : Transversal temperature profiles after 30,50, 100, 200, 500, 1000 2000 and 4000 years. The peaks in figures 43 correspond to the glass temperatures.

For this kind of HLW packages, the same observation can be done with cooler cells located in the periphery of the module. Maximum temperatures (blue for 1/2 cell, green for 1/2 slice, and 1/2 module) reached are higher simply related to the fact that the case is not geometrically optimized.

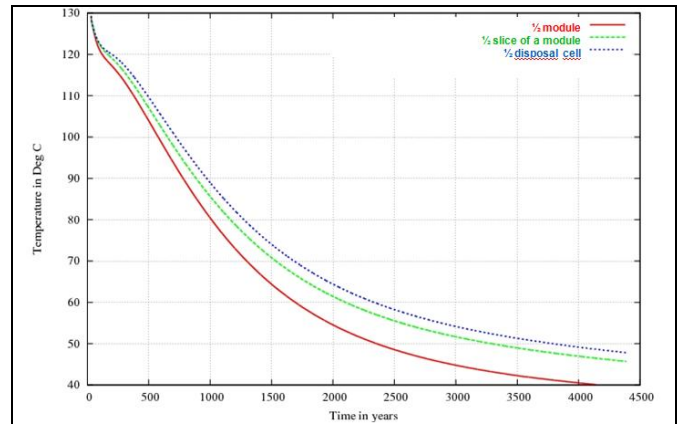


Fig. 36 : Maximum temperature evolution in the glass

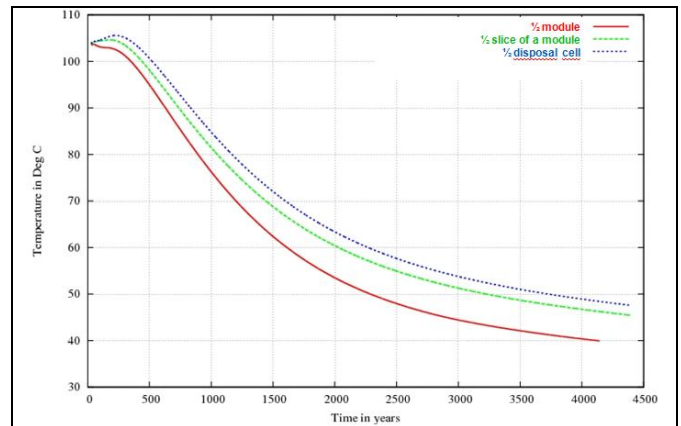


Fig. 37 : Maximum temperature evolution in over-pack

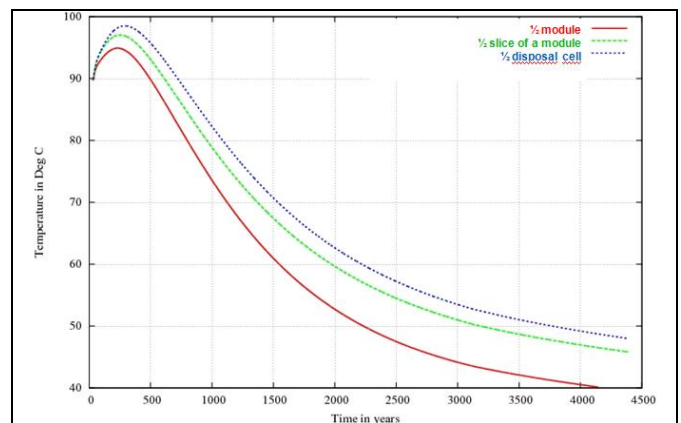


Fig 38. : Maximum temperature evolution in the clay

On Fig. 38, one notices that the peak temperature in the clay comes a long time (a few centuries) after filling of the access drifts. Thus, boundary conditions play a part in the clay peak temperatures reached as indicated more quantitatively in

table 2. This indicates clearly that limited domains used for optimization studies (see [1,2]) are conservative in the range of 4°C to 5°C at the peak. Moreover, one underlines that the thermal conservatism induced by a reduced domain can be much higher (up to 10°C) on periphery storage cells.

Table 2 : Peak temperature in the glass, over-pack and clay

	½ cell	½ slice of module	½ module
Glass	133.3 °C	133.3 °C	133.19 °C
Over-pack	105.5 °C	104.5 °C	104 °C
Clay	98.5 °C	97.3 °C	94.97 °C

CONCLUSION

This paper reports a theoretical thermal study done with the thermal code SYRTHES on a possible long live waste repository. This study focus on getting a better understanding of how strong the thermal conservatism of using a reduced domain for optimization studies can be.

To do so three domain extensions have been used (1/2 cell, half a slice of a module, and a complete half module leading to a very large mesh of 82 million tetrahedra handled thanks to parallelism). Results show that clay temperature surrounding cells located on the periphery are cooler than those located near the center of the module. This observation suggests that it could be interesting to put warmer packages in the periphery storage cells.

Two generic HLW waste kinds, with very different heat release transient have been calculated, one with a shape function representative of HLW packages coming from the reprocessing of PWR MOX, a second one illustrating what could be the shape function of HLW packages coming from the reprocessing of SFR MOX assemblies and including an important proportion of Americium.

For HLW packages characterized by early temperature peaks a domain limited to ½ a cell is completely adapted for optimization studies. For HLW packages characterized by late temperature peak wastes (SFR MOX type), taking into account a more extended domain (as it is partly done in [2]) seems interesting. Indeed, the large case underlines that optimizing on a reduced domain is clearly too conservative and that additional margins may exists.

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